Title: Simulations of Polymers with Brownian Dynamics
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Abstract: This work presents Brownian Dynamics simulations of macromolecules. A common approaches to hydrodynamic interactions employes the Rotne-Prager-Yamakawa (RPY) tensor. In such cases simple simulation step takes time proportional to $O(N^3)$ when Cholesky decomposition of RPY tensor is used. This makes the simulation too much time-consuming. This work proposes a new method for approximation of hydrodynamic interactions with a Toeplitz matrix. Decomposition of this matrix can be performed in $O(N^2)$ time, which considerably speeds up the simulations. In this work the new method was implemented, thoroughly tested, compared to a reference RPY approximation and applied to linear, cyclic and star macromolecules.

Keywords: Brownian dynamics, macromolecules, hydrodynamic interactions, Rotne-Prager-Yamakawa tensor, Toeplitz matrix, Cholesky decomposition